Benzo(a)acridine

Other names:	Benz[a]acridine
	7-Azabenz(a)anthracene
	1,2-Benzacridine
Inchi:	InChI=1S/C17H11N/c1-3-7-14-12(5-1)9-10-17-15(14)11-13-6-2-4-8-16(13)18-17/h1-11H
InchiKey:	JEGZRTMZYUDVBF-UHFFFAOYSA-N
Formula:	C17H11N
SMILES:	c1ccc2nc3ccc4ccccc4c3cc2c1
Mol. weight [g/mol]:	229.28
CAS:	225-11-6

Physical Properties

Property code	Value	Unit	Source
ie	8.10 ± 0.10	eV	NIST Webbook
log10ws	-6.65		Crippen Method
logp	4.541		Crippen Method
mcvol	178.230	ml/mol	McGowan Method
rinpol	397.83		NIST Webbook
rinpol	398.65		NIST Webbook
rinpol	398.74		NIST Webbook
rinpol	398.65		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	21.90	kJ/mol	402.80	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfust:	Enthalpy of fusion at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices